DYNAMAC
CORPORATION

~~Draft Report~~ Ad

O-PHTHALADEHYDE
Task 5: Product Chemistry Support
Registration Division

April 26, 1990

Contract No. 68-D8-0080

Submitted to:
Environmental Protection Agency
Arlington, VA 22202

Submitted by:
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The Dynamac Building
11140 Rockville Pike
Rockville, MD 20852

ORTHO-PHTHALALDEHYDE

PRODUCT CHEMISTRY SUPPORT

TASK 5

~~(Draft Report)~~ *Q1*

Submitter: Surgikos, Inc.

EPA File Symbol: 7078-RT

Pesticide Chemical Code: 129017

MRID(s): 412552-11 through -14, and 41267301

CAS Registry No.: 643-79-8

Chemical Name (Active Ingredient): 1,2-benzenedicarboxaldehyde

Common/Trade Name: ortho-phthalaldehyde/CIDEX OPA Antimicrobial

Use: Antimicrobial

INTRODUCTION

Surgikos, Inc. has submitted data (MRIDs 412552-11 through -14, and 41267301) for the registration of the 99% technical (T) formulation of the antimicrobial ortho-phthalaldehyde 99% T (EPA File Symbol 7078-RT). These data are being submitted in support of a new product registration. All product chemistry requirements pertaining to the technical grade of the active ingredient (TGAI) as described in 40 CFR §158.150 must be met to achieve full registration.

61-1. Product Identity and Disclosure of Ingredients

1,2-Benzenedicarboxaldehyde is the active ingredient in the 99% T registered to Surgikos, Inc.

Empirical Formula:	$C_8H_6O_2$
Molecular Weight:	134.13
CAS Registry No.:	643-79-8
EPA File Symbol:	7078-RT

The submitted product identity data (MRID 41255211) along with a Confidential Statement of Formula (CSF) reviewed in Confidential Appendix A satisfy the requirements of 40 CFR §158.155 regarding product composition for the Surgikos 99% T (EPA File Symbol 7078-RT). No additional data are required on this topic.

61-2. Beginning Materials and Manufacturing Process

The submitted data (MRID 41267301) reviewed in Confidential Appendix B satisfy the requirements of 40 CFR §158.160-162 (Guideline Reference No. 61-2) regarding beginning materials and the production process for the 99% T (EPA File Symbol 7078-RT). No additional information is required on this topic.

61-3. Discussion of the Formation of Impurities

Information (MRID 41267301) reviewed in Confidential Appendix C regarding formation of impurities does not satisfy the requirements of 40 CFR §158.167 (Guidelines Reference No. 61-3) for the 99% T (EPA File Symbol 7078-RT) because the registrant has not identified or explained the presence of a discernable peak on the submitted chromatogram; furthermore, no discussions were submitted pertaining to quality control, post-production reactions, and possible contamination from packaging materials. The following additional data are required:

- Following identification, the registrant must provide a discussion on the formation of an impurity present as a discernable peak on the submitted chromatogram. In addition, a discussion is required pertaining to quality control, post-production reactions, and possible contamination from packaging materials.

62-1. Preliminary Analysis

Data (1989; MRID 41255212) discussed in Confidential Appendix D do not satisfy the requirements of 40 CFR §158.170 (Guidelines Reference No. 61-1) regarding preliminary analysis of the Surgikos 99% T (EPA File Symbol 7078-RT) because an insufficient number of batches (four) were analyzed. In addition, a discernable peak on the submitted chromatogram with a concentration <0.1% of the TGAI was neither identified nor explained. Should this peak represent an impurity of toxicological concern, data will be needed. The following information is required:

- The registrant must provide preliminary analyses of at least five representative batches of the technical grade of active ingredient contained in the product to identify all impurities of toxicological significance associated with the active ingredient at any concentration, and all impurities present at ≥0.1% by weight of the TGAI. The preliminary analysis should be conducted at the point in the production process after which no further chemical reactions designed to produce or purify the substance are

intended. Complete and detailed descriptions of the methods used for sample analysis must be submitted, including statements of their precision and accuracy. The preliminary analysis report should include the identity and quantity of each ingredient for which analysis is conducted, along with the mean and relative standard deviation of the analytical results. Based on the preliminary analysis, a statement of the composition of the technical grade of active ingredient must be provided.

62-2. Certified Limits

Data reviewed in Confidential Appendix A (Confidential Statement of Formula dated 9/27/89) do not satisfy the requirements of 40 CFR §158.175 (Guidelines Reference No. 62-2) regarding certified limits for the Surgikos 99% T (EPA File Symbol 7078-RT) because the registrant has not explained how the proposed certified limits were obtained. The certified limits of this product appear to be based on preliminary analysis (see Confidential Appendix D). Since preliminary analysis data were determined to be inadequate (only four batches were analyzed) they may not be used to establish certified limits. The following additional data are required:

- The registrant must provide an explanation of how each certified limit was established (e.g., sample analysis using a validated analytical procedure, quantitative estimate based on the amounts of ingredients used, etc.).

62-3. Enforcement Analytical Methods

The submitted data (MRID 41255212) satisfy the requirements of 40 CFR §158.180 (Guideline Reference No. 62-3) regarding enforcement analytical methods for ortho-phthalaldehyde and its impurities. The method description and supporting data are presented in Confidential Appendix E. No additional data are required.

PHYSICAL AND CHEMICAL CHARACTERISTICS

The physical and chemical characteristics of the ortho-phthalaldehyde purified active ingredient (PAI) and technical grade of the active ingredient (TGAI) are summarized in Table 1.

The submitted data (1989; MRIDs 41255213, 41377501 and 41255214) ~~with one exception,~~ satisfy requirements of 40 CFR §158.190 (Guideline Reference No. 63-2 through 63-20) regarding physical and chemical characteristics. ~~Data concerning vapor pressure remain outstanding. The following additional data are required:~~

The registrant must submit data on vapor pressure.

Table 1. Physical and chemical properties of the ortho-phthalaldehyde 99% T (EPA File Symbol 7078-RT). Data are from MRID 41255213 unless otherwise indicated.

Guidelines Reference No., 40 CFR §158.190; Name of Property		Description [Method]
63-2.	Color	pale yellow to yellow
63-3.	Physical state	crystalline solid at 20°C
63-4.	Odor	sharp almond-like, characteristic of aromatic aldehyde compound
63-5.	Melting point	55-56°C [Mel-Temp apparatus]
63-6.	Boiling point	not required; ortho-phthalaldehyde T is a solid at room temperature
63-7.	Density, bulk density, or specific gravity	0.63 ± 0.10 g/mL at 20°C
63-8.	Solubility	

Solvent	Solubility at 20°C (g/100 mL)
water (deionized)	5
chloroform	20
acetone	20
di-isopropyl ether	3

63-9.	Vapor pressure	~~no data reported; registrant claims data for vapor pressure will be submitted by 2/90~~ 5.2×10^{-3} mm Hg at 21.0°C (MRID 413775-01)
63-10.	Dissociation constant	not required; ortho-phthalaldehyde is neither an acid nor a base and does not dissociate
63-11.	Octanol/water partition coefficient	$K_{o/w}$ = 26.8 at 1 C at 25°C $K_{o/w}$ = 22 at 0.1 C at 25°C [796.1550, 40 CFR] (data from MRID 41255214)

(Continued.)

Table 1. (Continued.)

Guidelines Reference No., 40 CFR §158.190; Name of Property	Description [Method]
63-12. pH	3.92-4.76 (diluted to 0.5% aqueous solution at 20°C)
63-13. Stability	ortho-phthalaldehyde T is stable at 25°C when protected from light; following storage in high-density polyethylene containers at elevated temperatures (37-40°C) for up to six months, the concentrations of ingredients are reported below:

	Month		
Component	0	3	6
ortho-phthalaldehyde	99.51	99.28	96.77
phthalide	0.24	0.21	0.20
pththalic anhydride	0.15	0.33	0.46
2-carboxybenzaldehyde	ND	0.06	2.48

the formation of 2-carboxybenzaldehyde results from the oxidation of one aldehyde group, while oxidation of both aldehyde groups gives phthalic anhydride; the packaging of the technical under an inert gas blanket of nitrogen or argon will prevent significant oxidation from occurring during prolonged storage at elevated temperatures; the technical product is expected to be sensitive to transition metal ions, which are known to catalyze the oxidation of aldehydes; when exposed to sunlight the technical product undergoes photochemical reactions to form phthalide and a dimer; when formulated with water, no photodegradation has been observed

63-14. Oxidizing or reducing action	no data reported
63-15. Flammability	not required; ortho-phthalaldehyde T is solid at room temperature

(Continued.)

Table 1. (Continued.)

Guidelines Reference No., 40 CFR §158.190; Name of Property	Description [Method]
63-16. Explodability	not required; ortho-phthalaldehyde T is not explosive on impact and does not contain any explosive ingredients
63-17. Storage stability	after storage in high-density polyethylene containers at 25 °C for up to six months, the concentrations (%) of ingredients are reported below:

	Month		
Component	0	3	6
ortho-phthalaldehyde	99.51	99.41	99.30
phthalide	0.24	0.20	0.18
pthalic anhydride	0.15	0.30	0.35
2-carboxybenzaldehyde	ND	ND	0.09

during storage stability testing, no significant physical changes were observed except for a slight tendency of the product to lump

63-18. Viscosity	not required; ortho-phthalaldehyde T is a solid at room temperature
63-19. Miscibility	not required; ortho-phthalaldehyde T is a solid at room temperature
63-20. Corrosiveness	ortho-phthalaldehyde T did not degrade the high-density polyethylene material used in the construction of commercial packaging during the 6-month long storage stability testing at 25 °C

Summary of Deficiencies

The product chemistry data requirements for this TGAI have not been satisfied. The following product chemistry requirements will have to be fulfilled:

61-3. Discussion of the Formation of Impurities

Following identification, the registrant must provide a discussion on the formation of an impurity present as a discernable peak on the submitted chromatogram. In addition, a discussion is required pertaining to quality control, post-production reactions, and possible contamination from packaging materials.

62-1. Preliminary Analysis

The registrant must provide preliminary analyses of at least five representative batches of the technical grade of active ingredient contained in the product to identify all impurities of toxicological significance associated with the active ingredient at any concentration, and all impurities present at ≥0.1% by weight of the TGAI. The preliminary analysis should be conducted at the point in the production process after which no further chemical reactions designed to produce or purify the substance are intended. Complete and detailed descriptions of the methods used for sample analysis must be submitted, including statements of their precision and accuracy. The preliminary analysis report should include the identity and quantity of each ingredient for which analysis is conducted, along with the mean and relative standard deviation of the analytical results. Based on the preliminary analysis, a statement of the composition of the technical grade of active ingredient must be provided.

62-2. Certified Limits

The registrant must provide an explanation of how each certified limit was established (e.g., sample analysis using a validated analytical procedure, quantitative estimate based on the amounts of ingredients used, etc.).

63-1 through 63-13. Physical and Chemical Characteristics

The registrant must submit data on vapor pressure.

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Attachments:
Confidential Appendices A through E

ORTHO-PHTHALALDEHYDE

PRODUCT CHEMISTRY REVIEW

TASK 5

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CONFIDENTIAL APPENDICES

Appendix A: 1 Page(s)
Appendix B: 1 Page(s)
Appendix C: 1 Page(s)
Appendix D: 1 Page(s)
Appendix E: 1 Page(s)

Confidential Appendices to the Scientific Review for the pesticide ortho-phthalaldehyde by the Registration Support Branch [Confidential FIFRA Trade Secret/CBI].

Page _____ is not included in this copy.

Pages 10 through 14 are not included in this copy.

The material not included contains the following type of information:

_____ Identity of product inert ingredients.

_____ Identity of product impurities.

✓ Description of the product manufacturing process.

_____ Description of quality control procedures.

_____ Identity of the source of product ingredients.

_____ Sales or other commercial/financial information.

_____ A draft product label.

_____ The product confidential statement of formula.

_____ Information about a pending registration action.

_____ FIFRA registration data.

_____ The document is a duplicate of page(s) _____.

_____ The document is not responsive to the request.

The information not included is generally considered confidential by product registrants. If you have any questions, please contact the individual who prepared the response to your request.